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FILE 'REGISTRY' ENTERED AT 14:06:11 ON 24 MAR 2009

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STRUCTURE FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

DICTIONARY FILE UPDATES: 22 MAR 2009 HIGHEST RN 1125392-64-4

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

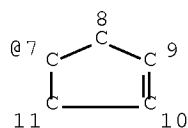
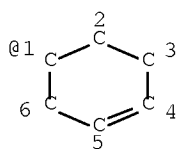
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<http://www.cas.org/support/stngen/stdoc/properties.html>

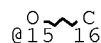
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L1 STR



G1 12

13
Ak
G2
14



VAR G1=1/7

VAR G2=X/15

NODE ATTRIBUTES:

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GGCAT IS SAT AT 13

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

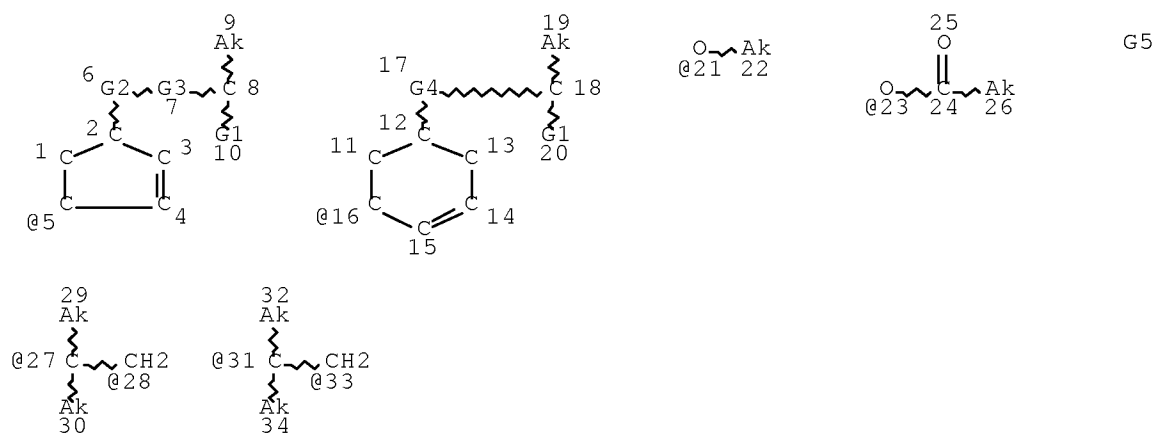
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L2 SCR 1992 OR 2021 OR 2016 OR 2026

L3 (41607)SEA FILE=REGISTRY SSS FUL L1 NOT L2

L4 STR



Page 1-A

35

Page 1-B

VAR G1=21/23

REP G2=(0-1) CH2

REP G3=(0-3) 27-6 28-8

REP G4=(0-3) 31-12 33-18

VAR G5=5/16

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 9

CONNECT IS E1 RC AT 19

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CONNECT IS E1 RC AT 32

CONNECT IS E1 RC AT 34

DEFAULT MLEVEL IS ATOM

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GGCAT IS SAT AT 30

GGCAT IS SAT AT 32

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L5 362 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

100.0% PROCESSED 41607 ITERATIONS

362 ANSWERS

SEARCH TIME: 00.00.01

=> d his

(FILE 'HOME' ENTERED AT 13:36:39 ON 24 MAR 2009)

FILE 'REGISTRY' ENTERED AT 13:36:55 ON 24 MAR 2009
ACT HUH779S2/A

L1 STR
L2 SCR 1992 OR 2021 OR 2016 OR 2026
L3 (41607)SEA FILE=REGISTRY SSS FUL L1 NOT L2
L4 STR
L5 362 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

FILE 'HCAPLUS' ENTERED AT 13:37:29 ON 24 MAR 2009

L6 2013 S L5
L7 QUE CAT# OR CATALYST?
L8 135 S L6 AND L7
L9 QUE LEWIS(N)ACID?
L10 5 S L8 AND L9

FILE 'REGISTRY' ENTERED AT 13:43:55 ON 24 MAR 2009

L11 219 S C7H11CL/MF
L12 63 S L11 AND DIENE
L13 16 S L12 AND 1-CHLORO

FILE 'STNGUIDE' ENTERED AT 13:54:52 ON 24 MAR 2009

L14 0 S L12 AND PENT?

FILE 'REGISTRY' ENTERED AT 13:58:20 ON 24 MAR 2009

L15 16 S L12 AND PENT?

FILE 'REGISTRY' ENTERED AT 14:01:02 ON 24 MAR 2009

L16 121 S L11 AND ENE
L17 0 S L11 AND 1-ENE
L18 5 S L11 AND PENTENE

=> fil hcap

FILE 'HCAPLUS' ENTERED AT 14:06:21 ON 24 MAR 2009
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FILE COVERS 1907 - 24 Mar 2009 VOL 150 ISS 13
FILE LAST UPDATED: 23 Mar 2009 (20090323/ED)

HCAplus now includes complete International Patent Classification (IPC)

reclassification data for the third quarter of 2008.

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<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d ibib abs hitstr hitind l10 1-5

L10 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2007:809821 HCAPLUS Full-text

DOCUMENT NUMBER: 147:322406

TITLE: Hydroalkoxylation of non-activated olefins catalyzed by Lewis superacids in alcoholic solvents: an eco-friendly reaction

AUTHOR(S): Lemechko, Pierre; Grau, Fanny; Antoniotti, Sylvain; Dunach, Elisabet

CORPORATE SOURCE: LCMBA UMR 6001, Institut de Chimie de Nice, Universite de Nice-Sophia Antipolis, CNRS, Nice, F-06108, Fr.

SOURCE: Tetrahedron Letters (2007), 48(33), 5731-5734

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:322406

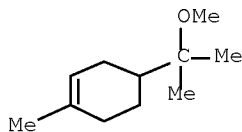
AB Lewis superacids such as tin(IV) triflate catalyze the intermol. addition of primary alcs. to non-activated olefins under mild conditions.

IT ~~14576-08-0P~~ 27153-54-4P ~~27153-57-7P~~

RL: SPN (Synthetic preparation); PREP (Preparation)
(hydroalkoxylation of non-activated olefins catalyzed by Lewis superacids in alc. solution)

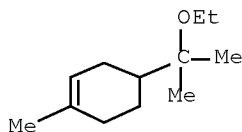
RN 14576-08-0 HCAPLUS

CN Cyclohexene, 4-(1-methoxy-1-methylethyl)-1-methyl- (CA INDEX NAME)



RN 27153-54-4 HCAPLUS

CN Cyclohexene, 4-(1-ethoxy-1-methylethyl)-1-methyl- (CA INDEX NAME)



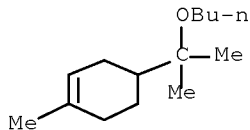
RN 27153-57-7 HCAPLUS

March 24, 2009

10/559,779

5

CN Cyclohexene, 4-(1-butoxy-1-methylethyl)-1-methyl- (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)
 Section cross-reference(s): 30
 ST olefin hydroalkoxylation Lewis superacid catalyst alc
 soln; ether prepn
 IT Addition reaction
 Addition reaction catalysts
 Alkoxylation
 Green chemistry
 (hydroalkoxylation of non-activated olefins catalyzed by Lewis
 superacids in alc. solution)
 IT Lewis acids
 Superacids
 RL: CAT (Catalyst use); USES (Uses)
 (hydroalkoxylation of non-activated olefins catalyzed by Lewis
 superacids in alc. solution)
 IT ~~14576-08-0P~~ ~~27153-54-4P~~ ~~27153-57-7P~~
 38376-28-2P 53767-86-5P 58195-90-7P 94281-60-4P 947701-74-8P
 947701-75-9P 947701-76-0P 947701-77-1P 947701-78-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (hydroalkoxylation of non-activated olefins catalyzed by Lewis
 superacids in alc. solution)
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L10 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2007:233179 HCAPLUS Full-text
 DOCUMENT NUMBER: 146:521952
 TITLE: An improved process for the preparation of the
 terpeneol esters
 INVENTOR(S): Sethi, Vijay Kumar; Singh, Samar; Dhar, Piary
 Lal; Taneja, Subhash Chandra; Thappa, Rajinder
 Kumar; Handa, Sukhdev Swami
 PATENT ASSIGNEE(S): Council of Scientific and Industrial Research,
 India
 SOURCE: Indian Pat. Appl., 13pp.
 CODEN: INXXBQ
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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IN 2000DE00663	A	20050805	IN 2000-DE663	200007
				18

PRIORITY APPLN. INFO.: IN 2000-DE663

200007

18

OTHER SOURCE(S): CASREACT 146:521952

AB The present invention relates to an improved process for the preparation of terpeneol esters. In the process terpinyl esters is prepared from pinenes (α - and β -pinenes) in a single step. The process gives only one isomer in major amts. i.e. α -terpinyl esters (50-55%) or other esters whereas the other isomers, β - & γ -terpeneol esters are formed only in 3.0-7.0% yield. The method involves the treatment for pinenes in an inert solvent with an acetylating agent containing a catalyst selected from the salts of group VIII, IIIA, II B or IB elements under low temperature conditions with vigorous agitation for a given time, separating the resulting reaction product by conventional methods and then separating the terpeneols esters by fractionation.

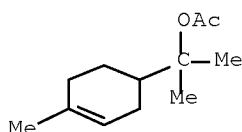
IT 80-26-2P, α -Terpinyl acetate 80-27-3P,
 α -Terpinyl propionate 2153-28-8P, α -Terpinyl
butyrate

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(improved process for the preparation of the terpeneol esters from
pinene)

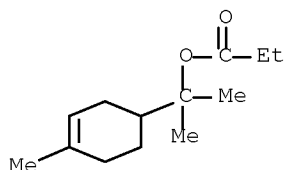
RN 80-26-2 HCAPLUS

CN 3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ -trimethyl-, 1-acetate
(CA INDEX NAME)



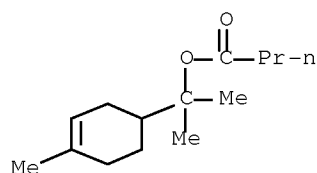
RN 80-27-3 HCAPLUS

CN 3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ -trimethyl-, 1-propanoate
(CA INDEX NAME)



RN 2153-28-8 HCAPLUS

CN Butanoic acid, 1-methyl-1-(4-methyl-3-cyclohexen-1-yl)ethyl ester
(CA INDEX NAME)



IC ICM C07C009-00
 CC 30-10 (Terpenes and Terpenoids)
 Section cross-reference(s): 62, 67
 IT Substitution reaction catalysts
 (acyloxylation catalysts; improved process for the
 preparation of the terpeneol esters from pinene)
 IT Lewis acids
 RL: CAT (Catalyst use); USES (Uses)
 (acyloxylation catalysts; improved process for the
 preparation of the terpeneol esters from pinene)
 IT Acids, uses
 RL: CAT (Catalyst use); USES (Uses)
 (inorg., acyloxylation catalysts; improved process for
 the preparation of the terpeneol esters from pinene)
 IT 7446-70-0, Aluminum chloride, uses 7447-39-4, Copper(II) chloride,
 uses 7487-94-7, Mercuric chloride, uses 7637-07-2, Boron
 trifluoride, uses 7646-85-7, Zinc chloride, uses 7664-38-2,
 Phosphoric acid, uses 7664-93-9, Sulfuric acid, uses 7705-08-0,
 Ferric chloride, uses 7720-78-7, Iron(II) sulfate 10043-35-3,
 Boric acid (H3BO3), uses
 RL: CAT (Catalyst use); USES (Uses)
 (acyloxylation catalyst; improved process for the
 preparation of the terpeneol esters from pinene)
 IT 80-26-2P, α -Terpinyl acetate 80-27-3P,
 α -Terpinyl propionate 2153-26-6P, α -Terpinyl formate
 2153-28-8P, α -Terpinyl butyrate
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (improved process for the preparation of the terpeneol esters from
 pinene)

L10 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1998:375712 HCAPLUS Full-text
 DOCUMENT NUMBER: 129:161726
 ORIGINAL REFERENCE NO.: 129:32915a,32918a
 TITLE: Palladium/tin catalyzed alkoxycarbonylation of
 naturally occurring bicyclic monoterpenes
 AUTHOR(S): da Rocha, Lilian L.; Dias, Adelson de. O.; dos
 Santos, Eduardo N.; Augusti, Rodinei;
 Gusevskaya, Elena
 CORPORATE SOURCE: Departamento de Quimica-ICEx, Universidade
 Federal de Minas Gerais, Belo Horizonte,
 31270-901, Brazil
 SOURCE: Journal of Molecular Catalysis A: Chemical
 (1998), 132(2-3), 213-221
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The alkoxy carbonylation of camphene and β -pinene has been studied. The following systems have been used as catalysts: PdCl₂(PPh₃)₂/SnCl₂/PPh₃ and PdCl₂(diphosphine)/SnCl₂/PPh₃ whose diphosphines were 1,2-bis(diphenylphosphino)ethane, 1,3-bis(diphenylphosphino)propane and 1,4-bis(diphenylphosphino)butane. It was observed that several concurrent transformations of monoterpenes occur in the reaction solns. To find the optimum conditions for alkoxy carbonylation the effect of the reaction variables on the product distribution has been investigated. The reaction of β -pinene exclusively yields the products of the Lewis acid catalyzed skeletal rearrangement accompanied by a nucleophilic addition of chloride and methoxy groups. No products of carbon monoxide incorporation were observed. Camphene was converted to the corresponding linear ester composed of approx. equal amts. of exo and endo isomers with a selectivity of 90% and virtually 100% regioselectivity (linear/branched esters) using a PdCl₂(PPh₃)₂/SnCl₂/PPh₃ system as a catalyst. Methyl bornyl ether was the only major byproduct. SnCl₂ and PdCl₂(PPh₃)₂ exhibited a strong synergetic effect on the camphene alkoxy carbonylation. PdCl₂(PPh₃)₂ alone showed a very low catalytic activity promoting the predominant formation of the thermodynamically more stable exo isomer (the exo/endo ratio is approx. 2:1).

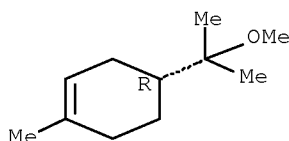
IT 30199-25-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(palladium/tin catalyzed alkoxy carbonylation of naturally occurring bicyclic monoterpenes)

RN 30199-25-8 HCAPLUS

CN Cyclohexene, 4-(1-methoxy-1-methylethyl)-1-methyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.



CC 30-10 (Terpenes and Terpenoids)

IT Alkoxy carbonylation

Alkoxy carbonylation catalysts

(palladium/tin catalyzed alkoxy carbonylation of naturally occurring bicyclic monoterpenes)

IT 99-85-4P 586-62-9P 4443-51-0P 5989-27-5P, (R)-(+)-Limonene

6120-13-4P 7785-26-4P 30199-25-8P 90976-73-1P

211237-72-8P 211237-79-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(palladium/tin catalyzed alkoxy carbonylation of naturally occurring bicyclic monoterpenes)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L10 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN

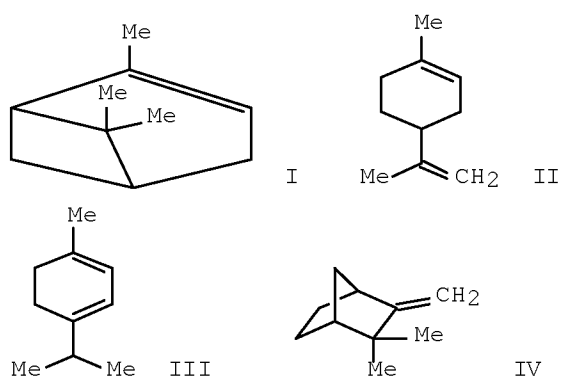
ACCESSION NUMBER: 1995:934321 HCAPLUS Full-text

DOCUMENT NUMBER: 124:56323

ORIGINAL REFERENCE NO.: 124:10661a,10664a

TITLE: PLS versus zeolites as sorbents and catalysts II. Terpene conversions in alumina-pillared clays and phosphates and medium

pore zeolites
AUTHOR(S): Stefanis, Adriana De; Perez, Giorgio; Ursini, Ornella; Tomlinson, Anthony A. G.
CORPORATE SOURCE: Istituto di Cromatografia, Area della Ricerca di Roma del C.N.R., C.P. 10 Monterotondo Staz., Rome, 00016, Italy
SOURCE: Applied Catalysis, A: General (1995), 132(2), 353-65
CODEN: ACAGE4; ISSN: 0926-860X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:56323
GI



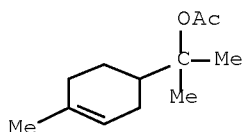
AB The reactions of α -pinene (I), limonene (II), and α -terpinene (III) in several alumina-pillared clays (PILCs) and a layered α -tin phosphate analog (Al-PILP) have been investigated under Lewis acid conditions and compared with the mid-pore zeolites USY, NH₄-ZSM-5 (with SiO₂/Al₂O₃ ratios = 35 and 235), and H⁺-mordenite. The bicyclic α -pinene gives the highest conversion, all catalysts giving >50% camphene (IV) at 100°C. Total yields show that USY is the strongest acid, after which the acidity order is: BP-PILC = ZSM-5 (35) > FAZA > H⁺-mordenite, and the layered phosphate appears to be less acid than the PILCs. No fenchene carbocation-derived products are produced, indicating that all the solids promote formation of the norbornyl cation intermediate. Selectivities in the unsubstituted PILCs is comparable with those in the zeolites (e.g. both FAZA and USY show selectivity against limonene production in the α -pinene reaction). BP-PILC also shows appreciable activity for α -pinene at 25°C (as does USY) whereas Al-PILP is inactive. Specific carbocation precursors are deduced from the product distributions and a 'carbocation cascade' based on pore acidity provides a rationalization of the results. However, site-selectivity effects do come into play in K⁺- and Ca²⁺-PILCs and it also appears that limonene occupies a specific site in USY. The reactions provide a means of generating terpene derived carbocations in the solid state.

IT 80-26-2P, α -Terpinyl acetate

RL: SPN (Synthetic preparation); PREP (Preparation)

(terpene conversions in alumina-pillared clays, phosphates, and medium pore zeolites)

RN 80-26-2 HCAPLUS

CN 3-Cyclohexene-1-methanol, $\alpha,\alpha,4$ -trimethyl-, 1-acetate
(CA INDEX NAME)

CC 30-10 (Terpenes and Terpenoids)

ST terpene rearrangement clay zeolite catalyst; mordenite
zeolite sorbent terpene rearrangement; alumina pillared clay
catalyst terpene rearrangement; camphene prepn terpene
rearrangement; pinene alpha conversion zeolite catalyst;
limonene conversion clay zeolite catalyst; terpinene alpha
conversion zeolite catalyst

IT Rearrangement

Rearrangement catalysts

Regiochemistry

(terpene conversions in alumina-pillared clays, phosphates, and
medium pore zeolites)IT 76-49-3P, Bornyl acetate 79-92-5P, Camphene ~~80-26-2P~~,
 α -Terpinyl acetate 99-85-4P, γ -Terpinene 99-87-6P,
p-Cymene 586-62-9P, Terpinolene 586-63-0P, Isoterpinolene
RL: SPN (Synthetic preparation); PREP (Preparation)
(terpene conversions in alumina-pillared clays, phosphates, and
medium pore zeolites)

L10 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:533566 HCAPLUS Full-text

DOCUMENT NUMBER: 121:133566

ORIGINAL REFERENCE NO.: 121:24137a,24140a

TITLE: Cycloadditions. 44.
2,3-Donor-acceptor-substituted 1,3-butadienes.
Synthesis by SO₂-extrusion from 3-sulfolenes and
Diels-Alder reactionsAUTHOR(S): Hoffmann, Ralf; Mattay, Jochen; Banning, Anja;
Rodewald, Ute; Moeller, Manfred M.CORPORATE SOURCE: Org. Chem. Inst., Univ. Muenster, Muenster,
GermanySOURCE: Journal fuer Praktische Chemie/Chemiker-Zeitung
(1994), 336(4), 343-9

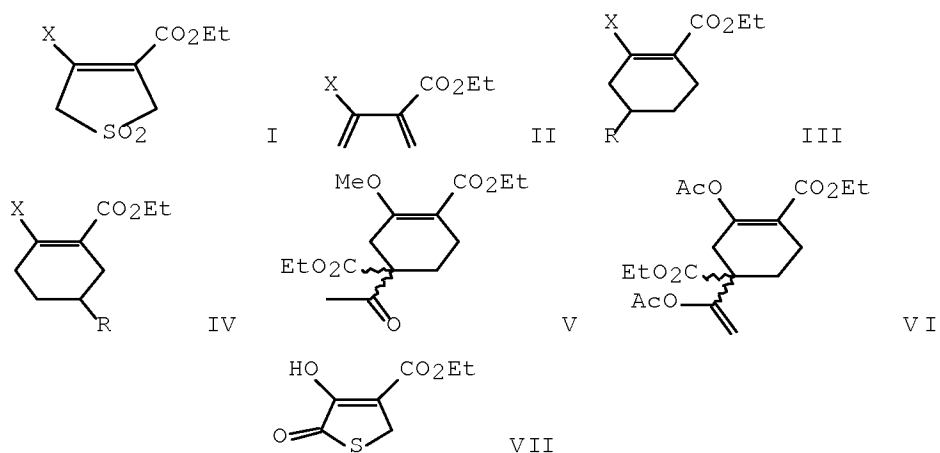
CODEN: JPCCEM; ISSN: 0941-1216

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:133566

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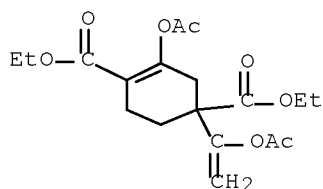
AB The thermal extrusion of SO₂ from disubstituted 3-sulfolenes I (X = OMe, OAc) leads to 2,3-donor-acceptor-substituted 1,3-butadienes II. These dienes react with acrylic acid ester and Et vinyl ether to the corresponding Diels-Alder adducts III and IV (R = CO₂Et, OEt) and with themselves to the cyclic dimerization products V and VI. The regiochem. of the cycloadducts has been determined by chemical- and NMR-methods. The pyrolysis of 3-sulfolene I (X = OH) afforded the thiolactone VII whose structure has been verified by x-ray diffraction anal. In addition, the influence of Lewis acid catalysts on the Diels-Alder reaction and an approach to transition state calcn. by means of the semiempirical AM 1 method has also been investigated.

IT 157163-35-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 157163-35-4 HCAPLUS

CN 1-Cyclohexene-1,4-dicarboxylic acid,
2-(acetyloxy)-4-[1-(acetyloxy)ethenyl]-, 1,4-diethyl ester (CA
INDEX NAME)



CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 75

ST donor acceptor butadiene Diels Alder regiochem; sulfolene conversion
donor acceptor butadiene; Lewis acid Diels Alder
catalyst; transition state Diels Alder; thiolactone

IT Diels-Alder reaction catalysts

(Lewis acids, inducing self-Diels-Alder

reaction of 2,3-donor-acceptor-substituted 1,3-butadienes)

IT Lewis acids

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalysts inducing self-Diels-Alder reaction of
2,3-donor-acceptor-substituted 1,3-butadienes)
IT 7446-70-0, Aluminum chloride, uses 7550-45-0, Titanium
tetrachloride, uses 7646-85-7, Zinc chloride (ZnCl₂), uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for self-Diels-Alder reaction of
donor-acceptor dienes)
IT 16205-98-4P, 3-Oxocyclohexanecarboxylic acid 95992-17-9P
157163-29-6P 157163-30-9P 157163-31-0P 157163-32-1P
157163-33-2P 157163-34-3P ~~157163-35-4P~~ 157163-36-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

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